

MOMENT ANALYSIS OF TERTIARY PROTEIN STRUCTURES

5 Abstract of the Disclosure

Techniques for analyzing protein structures, such as a tertiary protein structure, are provided. A centroid of the residue centroids is calculated. The centroid of the residue centroids is used as a spatial origin of a global linear hydrophobic moment. The correlation between residue centroid magnitude and residue solvent accessibility is
10 enhanced. The global linear hydrophobic moment is defined, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment. A method for comparing at least two tertiary protein structures is also disclosed.